Atomic Imaging of Light Elements: Nitrogen in Gallium Nitride

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The One-Ångstrom Microscope, a new generation of high resolution instruments, enables NCEM scientists to investigate solids that contain light elements such as C, N and O with mono-atomic resolution. For the first time a full reconstruction of the electron wave at the exit surface of a GaN sample is achieved, separating N and Ga columns with a spacing of 1.13Å at a cubic / hexagonal interface. This result is based on the combination of electron optical performance with advanced computer processing and demonstrates that light elements such as N can be observed at ultra-high resolution with coherently scattered electrons.

Background – Atomic resolution imaging of light elements such as carbon, nitrogen or oxygen by electron microscopy is a major challenge. Despite substantial recent progress, quantitative imaging of light elements has remained elusive, especially in the presence of heavy atom neighbors found in large band-gap semiconductors or superconducting oxides. The low electron-scattering power of light elements and their small covalent radius (<1.5Å) requires major advances in the performance of electron-optical instrumentation. As a result, superconducting oxides and hard materials such as diamond, sapphire, silicon nitride or gallium nitride have resisted investigation at a mono-atomic level. Overcoming this barrier is of substantial scientific and industrial interest because of the engineering or physical properties of superconductors, ceramics and semiconductors.

Accomplishment – NCEM scientists have demonstrated that the outstanding information limit of its One-Ångstrom Microscope (OÅM), a 300kV field emission instrument coupled with advanced computer processing, can be exploited to access information from the sub-Ångstrom domain, even for light elements. Single lattice images of C-C "dumbbells" in diamond were recorded, proving 0.89Å information transfer. However, the interference pattern that forms an image in an ultra-high resolution field- emission microscope can be confusingly complex. Advanced computer processing of a series of such images is required to provide a simple ultra-high resolution image.

Figure 1 is a comparison between previous and present capabilities using the interface between hexagonal (2H) and cubic (3C) gallium nitride. The micrograph at the left was recorded with the Atomic Resolution Microscope which until recently had the best information limit nationwide. The micrograph at the right was recorded with the One-Ångstrom Microscope and contains sub-Ångstrom details from the interface. However, localization of atomic columns is impossible from such a single micrograph.

Figure 2 depicts the same interface produced by computer processing of a through-focal series of 20 images from the OÅM to unscramble the amplitudes and phases of the electron wave. The resulting phase image of the electron exit wave shows that gallium and nitrogen columns can be unambiguously distinguished by their contrast, and are clearly resolved at their separation of 1.13Å. The ac,ac,... stacking of the hexagonal phase transforms into the abc,abc,abc,.. stacking of the cubic phase at the 2H/3C interface.

In summary, coherently scattered electrons were used for the first time to resolve all the atomic columns, *including nitrogen*, in GaN. To obtain the final image, amplitudes and phases of the electron exit wave were reconstructed, with a resolution of better than 1.13Å, from a focal series of 20 lattice images, each containing information from the sub-Ångstrom regime.

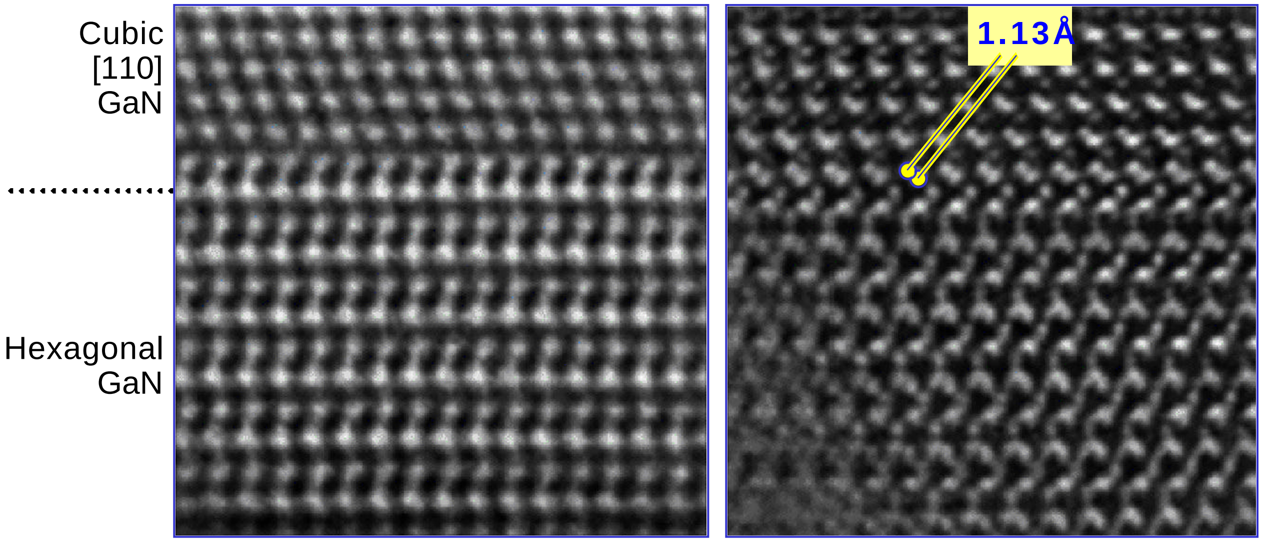

Fig.1: High-resolution micrographs of interface between cubic (3C) and a hexagonal (2H) GaN recorded along the (110)/(11$\bar{2}$0) zone axis. Left: Image from the NCEM Atomic Resolution Microscope with information limit of 1.4Å shows Ga positions. Right: Image from the NCEM One-Ångstrom Microscope with information limit of better than 0.9Å shows sub-Ångstrom spacings.

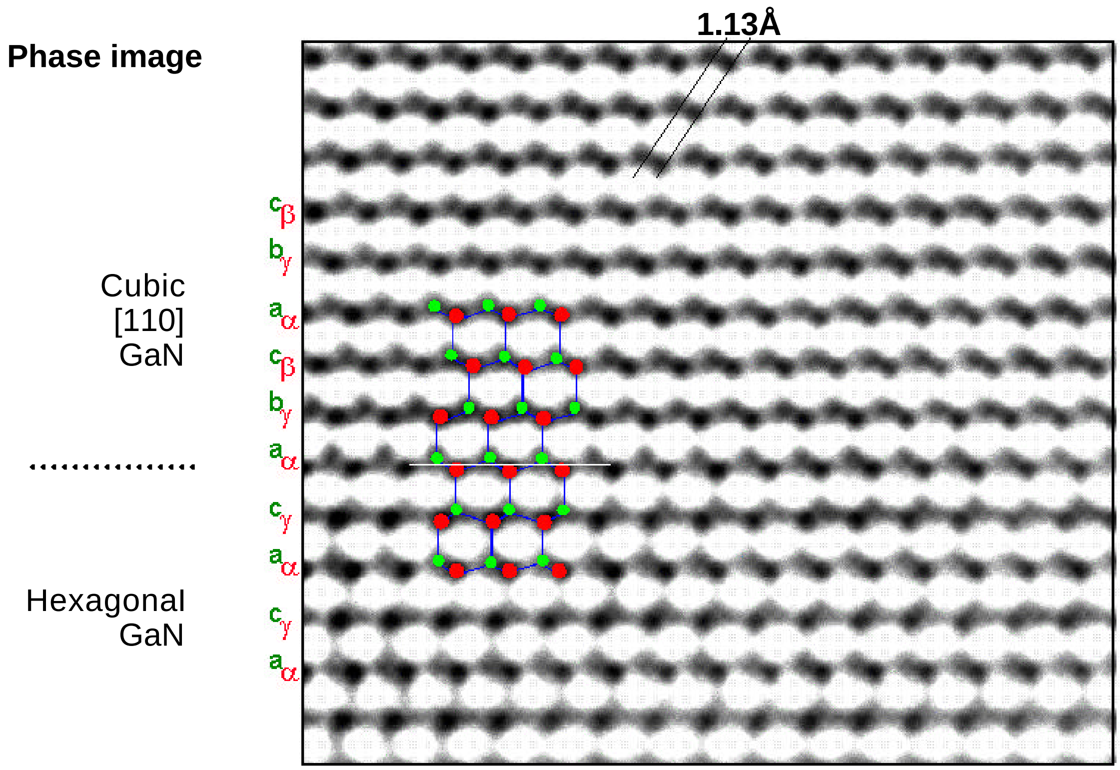

Figure 2: Reconstruction of the phase of the electron exit wave from the 3C/2H interface shown above. The reconstruction used a focal series of 20 images from the One-Ångstrom Microscope. Ga and N sub-lattices are clearly resolved at a separation of 1.13Å, and are distinguished by the different contrast at the (darker) Ga and (lighter) N sites that is maintained across the interface.